**Institution: 10007822**

**Unit of Assessment: 12**

**Title of case study: Improved shock physics modelling as an alternative to nuclear testing**

**1. Summary of the impact** (indicative maximum 100 words)

Cranfield University's research in computational fluid dynamics (CFD), turbulence models, studies of instabilities and the development of multi-scale methods has reduced the computational uncertainty in the modelling and simulation used by the Atomic Weapons Establishment (AWE) to support the safety and performance of nuclear weapons.

Cranfield's research in compressible turbulent flow for Low Mach numbers is now employed to increase accuracy in CFD codes employed by the German Aerospace Agency DLR, Pennsylvania State University, and the French Commissariat a l'Energie Atomique, which use this work to model flows ranging from turbulent mixing through inertial confinement fusion (ICF) to scramjets.

**2. Underpinning research** (indicative maximum 500 words)

Now that it is no longer possible to conduct live tests of nuclear weapons, accurate computer modelling is essential to underwrite their safety and performance. Modelling to understand instabilities and turbulent mixing at material interfaces is an area that demands better understanding.

Cranfield's work on CFD (2004 to date) concerns:

- the development of computational fluid dynamics methods, turbulence models and engineering physics studies of instabilities (Richtmyer-Meshkov and Rayleigh-Taylor) and compressible turbulent mixing; and
- development of multi-scale methods and study of dynamic friction across material interfaces.

The research is motivated by a range of diverse applications in science and engineering, including: inertial confinement fusion (ICF); micro and nanocrystalline materials and interfacial friction in materials; nuclear energy; detonation; supersonic combustion; and astrophysics.

In ICF, the main area of application of the research, the dense shell, filled with deuterium-tritium (DT) gas, implodes when irradiated by laser beams or by other means. When a shock wave refracts through the shell-fuel interface, the boundary experiences Richtmyer-Meshkov instability (RMI). RMI leads to the growth of perturbations on the shell-fuel interface and causes turbulent mixing of the materials. Rayleigh-Taylor instability (RTI) and mixing also occurs at the shell-fuel interface towards the end of the implosion phase, when the less dense gas decelerates the shell. RMI and RTI turbulent mixing reduce the heating of the gas during the implosion phase and inhibit the thermonuclear reaction after ignition, degrading the performance of the ICF target. Accurate modelling of RMI and RTI is a major uncertainty in calculating how an ICF target will behave.

In the framework of the present research, Cranfield developed new high-resolution and high-order computational methods that improve the accuracy in compressible turbulent mixing simulations [P1, P2, P3]. The results from the simulation and modelling studies were validated against specially designed experiments performed at AWE, as well as simulation and modelling data using AWE's industrial codes. Cranfield investigated the influence of the initial conditions on RMI, RTI and turbulent mixing in a range of ICF mixing problems.

In the course of the research [P4, P5], Cranfield also developed multi-scale models that couple continuum and molecular dynamics methods in order to study dynamic friction between material interfaces. Friction at the interface between dissimilar metallic components as a result of high velocity impact or explosive loading can have a profound effect on the subsequent motion. A comprehensive understanding of the processes involved across a wide range of initial conditions is still not available. This research revealed the growth of epitaxial layers of the softer material, shifting of the sliding interface due to formation of shear-bands, development of amorphous structures, and ultimately the resultant motion of the components. Analysis of the results also linked these processes to the changes in the state of the material through growth of dislocations and thermal effects [P5].

The research enhanced our understanding in compressible turbulent mixing and dynamic friction, which are core activities of AWE's technical programme.

| Key Researchers | Post details | Dates involved | Research |
|---|---|---|---|
| Dr Ben Thornber | Research Fellow/Lecturer | 2004 - 2013 | Compressible turbulent mixing, CFD |
| Dr Marco Hahn | Research Fellow/Lecturer | 2004 - 2010 | Compressible turbulent mixing, CFD |
| Prof Dimitris Drikakis | Professor | 2003 - present | Turbulent mixing, CFD, multi-scale modelling, dynamic friction, engineering turbulence modelling |

**3. References to the research** (indicative maximum of six references)

***Evidence of quality – Peer Reviewed Journal Papers***

P1 M Hahn, D Drikakis, D L Youngs and R J R Williams, "Richtmyer-Meshkov turbulent mixing arising from an inclined material interface with realistic surface perturbations and reshocked flow", Physics of Fluids, **23**, p. 046101 (11 pages), 2011.
DOI: 10.1063/1.3576187

*P2 B Thornber, D Drikakis, D L Youngs[a] and R J R Williams[b] "The influence of initial conditions on turbulent mixing due to Richtmyer–Meshkov instability", Journal of Fluid Mechanics, **654**, pp. 99-139, 2010.
DOI: 10.1017/S0022112010000492

*P3 B Thornber, A Mosedale, D Drikakis, D Youngs[a] and R J R Williams[b], "An Improved Reconstruction Method for Compressible Flows with Low Mach Number Features'', Journal of Computational Physics, **227,** pp. 4873-4894, 2008.
DOI: 10.1016/j.jcp.2008.01.036

*P4 P Barton, B Obadia, and D Drikakis, "A conservative level-set based method for compressible solid/fluid problems on fixed grids", Journal of Computational Physics**, 230**, pp. 7867-7890, 2011.
DOI: 10.1016/j.jcp.2011.07.008

P5 P T Barton, M Kalweit, D Drikakis and G Ball "Multi-scale analysis of high-speed dynamic friction", Journal of Applied Physics, **110**, p. 093520 (8 pages), 2011.
DOI: 10.1063/1.3660194

*       3 identified references that best indicate the quality of the research

Key to co-authors
a, b: AWE, Aldermaston, UK.

***Further evidence of quality – underpinning research grants***

G1 AWE William Penney Fellowship, total £263K: *Advanced Turbulence Modelling for Compressible Turbulent Mixing* £135k, 04/2008-03/2011 and £128k, 01/2012-12/2014, Prof Drikakis for his contributions to computational science, fluid dynamics and materials in relation to design physics, aerospace and defence.

G2 EPSRC (EP/C515153) and MoD-AWE Joint Grant Scheme (JGS 971) *Computational and Theoretical Modelling of Shock-Induced Instability and Mixing across Material Interfaces*, £242,609, 10/2005-01/2009. PI: Prof Drikakis

G3 EPSRC (EP/D051940/1) and MoD- AWE Joint Grant Scheme (JGS 607) *Multiscale Modelling of Meso and Nano Scale Interfacial Dynamics Phenomena*, £249,728, 02/2006-10/2009. PI: Prof Drikakis

**4. Details of the impact** (indicative maximum 750 words)

*Due to the nature of AWE's work, focused on nuclear weapons, national security makes it impossible to provide accessible published evidence of the impact of Cranfield's research. What we can provide, detailed below, is an explanation of the context in which the work has been applied, and quotes from senior individuals at AWE, attesting to the impact of this research on their work.*

Accurate computer modelling is needed to underwrite the safety and performance of nuclear weapons. Instabilities and turbulent mixing at material interfaces is one area where better understanding is essential [C1]. A decade ago, the type of "Large Eddy Simulation" used at AWE to gain a fundamental understanding of the mixing processes was much criticised by the academic community with respect to its ability to capture accurately the correct turbulent-flow physics.

The numerical methods developed at Cranfield University have been used by AWE to investigate the influence of initial conditions of mixing due to Richtmyer-Meshkov instability. Turbulence modelling simulations often ignore the influence of initial conditions on turbulent mixing, so Cranfield's work has a substantial impact in reducing computational uncertainty in turbulent mixing predictions and is now taken into account in AWE's modelling.

*"The collaboration between AWE and Cranfield University, which has involved simulation methods at both institutions and experiments at AWE, has led to a high degree of confidence in the computer modelling we now use to understand turbulent mixing*." [C2, C4]

The methods developed at Cranfield have also been used for 3D simulation of complex flows where mixing is on average two-dimensional. These results have led to a substantial advance with respect to validation and verification of computational models by improving the accuracy of engineering turbulence models (Reynolds-Averaged Navier-Stokes models) used in ICF applications at AWE.

During the course of this research, a key improvement was made by Cranfield to the Godunov methods used at Cranfield to simulate compressible turbulent flow, in particular the behaviour at low Mach number. This improvement significantly increases the accuracy of computational fluid dynamics (CFD) codes in turbulent flow simulations. Furthermore, it enhances the efficiency of CFD codes because high accuracy can be attained even with low numerical grid resolution, thus leading to shorter computing times.

Low-Mach corrections developed at Cranfield – as well as variants of Cranfield's work produced by other research groups – are now employed in CFD codes in the German Aerospace Agency DLR [C5], Pennsylvania State University [C6] and the French Commissariat a l'Energie Atomique [C7]. These organisations use these CFD codes for flows ranging from turbulence mixing through to scramjets.

Cranfield's work has inspired further developments in the international research community, eg, the French nuclear hydraulics code FLICA-OVAP and at Tsinghua (China) in relation to turbine blades

A related area of physics that is also of concern to AWE is dynamic friction at material interfaces under extreme conditions of velocity and normal stress. AWE's previous modelling using continuum hydrocodes, and work at the US Los Alamos National Laboratory (LANL) using molecular dynamics simulations, had produced conflicting predictions of behaviours in this regime. AWE resolved this by adopting Cranfield's approach and has incorporated this in model development.

> *"Research performed by Professor Drikakis' group led to the development of a hybrid method in which continuum and molecular dynamics codes were directly coupled. This approach has helped to reconcile apparent contradictions in the earlier work, and has provided new insights that will inform future model development at AWE." [C3]*

**5. Sources to corroborate the impact** (indicative maximum of 10 references)

C1 K O'Nions, R Pitman, C Marsh: "Science of nuclear warheads", Nature, 415, 853-7, 2002

C2 Contact: Distinguished Scientist, AWE Aldermaston, UK

C3 Contact: Division Manager, AWE Aldermaston, UK

C4 Contact: Team Leader, AWE Aldermaston, UK

C5 Contact: Research staff, DLR, Braunschweig, Germany

C6 Contact: Research Associate, Navy Research Laboratory, USA

C7 Contact: Research Scientist, Atomic Energy and Alternative Energy Commission (CEA), France